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14. ABSTRACT

- Development of new quantum theory for the accurate description of molecular structure and spectra

- Implementation of this new theory into general purpose computer programs (ACES II) to make it possible for many investigators, besides ourselves, to readily apply these new methods to problems of their interest

- (3) Application of these new methods to high energy, density molecules, assessing their energy content, stability, possible synthetic paths, activation barriers, and providing spectroscopic fingerprints for identification.

Section II summarizes some of the highlights of our work for the past two years. The references refer exclusively to the recent papers published under this grant, listed in Section III. Section IV shows the invited presentations assisted by this grant. Sections V and VI report the students and postdocs supported under this work and the recognition's we've received.

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On

Metastable Molecules in Ground and Excited States:

Theory Development, Implementation and Applications

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Contents

I. Objectives

Our work for the AFOSR has three primary components:

♦ Development of new quantum theory for the accurate description of molecular structure and spectra

♦ Implementation of this new theory into general purpose computer programs (ACES II) to make it possible for many investigators, besides ourselves, to readily apply these new methods to problems of their interest

♦ (3) Application of these new methods to high energy, density molecules, assessing their energy content, stability, possible synthetic paths, activation barriers, and providing spectroscopic fingerprints for identification.

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II. Summary of Accomplishments - 9/99-9/00

Our work combines critical methodological developments with their application to energetic molecules. This allows us to suggest several new, experimentally unknown species that according to predictive theory have sufficient energy storage and activation barriers that they can be made under some circumstances. In this sense, quantum chemistry offers a screening mechanism for prospects, consistent with the HEDM program's search for evolutionary and even revolutionary concepts on how to obtain greater usable energy from metastable molecules and other scenarios. However, because most of these molecules are unknown experimentally, if they are to be made and identified, we require predictive information about their spectroscopic characteristics, meaning IR-Raman, UV-vis, UPS, NMR, ESR, and other kinds of spectroscopy. Quantum chemistry thus needs to provide those results as well, which means that new, more accurate methods have to be developed. Under this program, we have developed coupled-cluster (CC) methods for all the above kinds of spectroscopy.

Nowadays, CC theory is widely recognized as being the most accurate, widely applicable quantum chemical method. With its generalization to analytical gradients to provide forces, and whose differences provide force constants, we obtain molecular structure, transition states and activation barriers, and associated vibrational spectroscopy. Since not all effects important to HEDM molecules are limited to the electronic ground states, CC extensions to excited states, via the equation-of-motion (EOM-CC), its generalizations for ionized states, IP-EOM-CC and DIP-EOM-CC (double ionization potential), and electron attached states, EA-EOM-CC; further generalizations to the similarity transformed, STEOM-CC for excited states, and EOM-CC methods for NMR, for Raman intensities, and for excited state properties, provide a unified, very accurate group of tools for the description of ground and

excited states. All of these have been developed in this program over the last decade. Their incorporation into ACES II makes their application routine today, and many of the investigators in this program have successfully used the program for their own studies. Developments of the type summarized here occur over a number of years, but each year has its highlights, some of which are summarized below.

A. CC Theory -- Though CC theory is the most accurate method that can usually be applied to small molecules, we continue to seek even more accuracy from the CC framework. Last year, one of our principal accomplishments was our introduction of connected quadruple excitations (ie T_4) into CC theory in a way that was no more demanding that the full treatment of triple excitations, T_3 [7]. This allowed us to get the vibrational frequency of N_2 to ~1 cm^{-1} [14]. However, when we did the same type of calculation for O_3[17], a notoriously difficult case, we concluded that pentuple excitations, T_5, could not be dismissed. This year we have made the initial inclusion of the connected pentuple operator, T_5 [33]. In comparison with full CI reference values, this reduces the average error for several molecules from 1.44 mH for CCSDT to 0.125 mH for CCSDTQ, all the way to 0.022 mH, an order of magnitude improvement. A factorized version of T_5 will be implemented to make such calculations including Q and P almost as common as those with none iterative inclusion of triples, like CCSD[T] or CCSD(T).

B. Using the factorized approach, we have also studied a series of molecules with triple bonds, where the correlation effects are most pronounced [39]. These are large scale calculations of structures, vibrational frequencies, energetics, all with T_5. This study documents the numerical significance of T_5 for a variety of examples.

C. Continuing on this theme, we also wrote and applied a full CI program, to investigate a number of potential CC approximations which would be nearly impossible to consider if general programs were to be written. In this way, we reported the first treatment of CC theory through hextuple, septuple, and octuple excitations, ie CC(8) [34]. This allows us to study the convergence of CC theory through CC(8), as well as MBPT through 20th order, and compare to full CI. For cases where MBPT diverges, we resumed the energies using rational approximations (Pade' approximants), demonstrating that there was no fundamental problem with the diverging MBPT series that resummation could not cure, since all the information is contained in the MBPT series. Of course, CC theory converges much more rapidly than CI, exhausting the full CI values to sub MH accuracy at CC(5), which is consistent with the study of pentuples in A above, where a more general purpose program was written.

D. Using the same full CI strategy, we also investigated very high level EOM-CC methods. We report the first full EOM-CCSDT results, as well as EOM-CC(4), EOM-CC(5), and EOM-CC(6)[37]. The full EOM-CCSDT is significantly different from the highest previous level done, EOM-CCSDT-3 [11] for states dominated by double excitations. This attests to the requirements for excited states that will embrace all kinds, singly and doubly excited, Rydberg, and charge transfer. The goal of excited state theory is to offer an unambiguous procedure that depends only upon basis set and level of excitation to reliably describe all types of excitations. These studies quantify that.

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E. Finally, using the same procedure we have recently investigated the IP-EOM-CC methods for ionized and EA-EOM-CC for electron attached states [38], again going to much higher excitation levels than would be practical in a general purpose program and exploring the differences in the convergence of the ground and the ionized states. That latter might point to superior but practical methods constructed from treating the reference state and the ionized, electron attached, or excited states at different levels.

F. Theory for extended systems -- In another developmental effort, we consider the theoretical description of extended systems like polymers, films, or solids, which is the form that most fuels will assume. To do such studies theoretically requires that periodic boundary conditions be imposed. This fundamentally changes the implementation of quantum chemical methods that are normally applied to isolated molecules, as unlike a molecule, infinite periodic systems have the property that the wavefunction never goes to zero. In practice, DFT is usually the choice for such 'solid state' applications, but DFT does not offer a path toward converging to the right answer as do ab initio correlated methods like CC/MBPT theory. Hence, a great deal can be gained by developing correlated wavefunction methods for such periodic systems. The fact that this has not been done attests to its difficulties. In two studies [23,32] we addressed the particularly difficult topic of excited states in polymers.

G. NMR Coupling Constants -- In addition to the above theory developments, we have spent sometime with the fascinating issue of coupling constants across H bonds in NMR. With reference to HEDM, predicted NMR spectra was instrumental in the identification of N_5^+, accomplished by use of the ACES II program, and the NMR parameters have been reported by us for experimentally unknown N_5^- [26], which is likely to be the next target for synthesis. Furthermore, in several scenarios for embedding atoms like C, N, and B in solid hydrogen to increase energy storage, the formation and detection of such H bonds are pertinent. In a series of three communications to JACS [30, 31, 35] and one to the JPC [40], we have used our predictive CC methods for NMR coupling constants to explore and predict the values that could be observed for coupling constants in H bonded situations between N, O, F, and P atoms. We show that the principal determinant of the value is the distance between the atoms, and secondly, the type of H bond which involves, among other issues, whether the structure is charged or neutral. We have shown that structure determinations in large biological molecules can be greatly accelerated from the correlation between coupling constants and distance that we have established for N-H-N bonds [35]. Previously, the position of H bonds could not be established by X-ray structures, yet coupling constants are now known to provide 'fingerprints.' With our work, they do not only provide 'fingerprints' but actually tell you the bond lengths involved to a high accuracy.

H. Polynitrogen Systems -- In a review of several years work on "polynitrogen molecules that don't exist but should", I summarize work on exploring potential nitrogen molecules that theory says should exist under some circumstances, by virtue of their activation barriers and other properties [29]. As only N_2 and N_3 were known until recently with Christie's synthesis of N_5^+, the prospects for making other systems is quite fascinating. In this paper I emphasize the essential role that the pentazole

anion, N_5^- should have, its stability, and energetics, and call for its synthesis. Furthermore, we have supplied its Raman and IR spectra, plus NMR parameters, to identify it once it is made [26].

I. Ab Initio DFT -- Below and elsewhere [43] I discuss the philosophy of Ab Initio DFT, but the most important next step is to obtain a correlation potential from the simplest wavefuntion correlation method, MBPT(2). We present such a formula in a communication to the JCP [41] that will appear shortly. We have also initiated some numerical studies of this formula and its variants.

Summary of Accomplishments - 9/98-9/99

A. In a notable achievement, we have introduced a factorized evaluation of T_4 that requires only a ~n^7 evaluation, [7] which is the same as the non-iterative approximations [T] and (T). Using a converging series of basis sets, cc-pVNZ, we determine that the effects of (Q), as measured by the CCSDT(Q_f) model is 19 cm^{-1} for the harmonic vibrational frequency of N_2 [14]. These calculations used up to 182 contracted Gaussian functions, which attest to the efficiency of our CCSDT implementation and the ease of evaluation of the T_4 contribution. In the absence of the (Q_f) effect, the harmonic frequencies would have an error of this order. With the Q_f effect, we show that the computed vibrational frequency is within 1 cm^{-1} of experiment.

B. Just as the non-iterative (Q_f) approximation well reproduces the full effects of the non factorized (Q), which is an ~n^9 method instead of ~n^7, the results of the iterative CCSDTQ-1 method are well reproduced by the factorized equivalent, CCSDTQ$_f$-1, which, today, offers benchmark results in the absence of the full CI limit [7]. In prior work, we have shown that CCSDTQ-1 is usually quite close to the full CCSDTQ, which is virtually the full CI when those results are available.

C. One of the most demanding problems that has been encountered in electronic structure theory is a correct description of the vibrational frequencies of the ozone molecule. O_3 is of interest as a component of a novel HEDM system, since burning fuels with ozone instead of O_2 provides a greater energy release. From another viewpoint, if the molecule could be trapped in its equilateral triangular excited state, significantly more energy could be produced. However, even the ground state of ozone is difficult to accurately describe. In a series of prior efforts (summarized in reference [1]), it has been shown that the full CCSDT basis set limit for ozone would give errors of about 50 cm^{-1} for the symmetric stretch, 50-60 cm^{-1} for the asymmetric stretch, and 15 cm^{-1} for the symmetric bend. Hence, the role of T_4 is critical. With adequate basis sets it would be impossible to include T_4 without our factorization approximation [17]. Hence, we applied our CCSDT(Q_f) approximation to this problem. For the symmetric stretch, we obtain agreement to just 2 cm^{-1}, while for the bend the difference is -7 cm^{-1}. For the very hard to describe asymmetric stretch, the effect of Q_f is significant, reducing the error by better than half to 23 cm^{-1}. No other CC or CI method can claim better accuracy.

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D. In another methodological development, we introduced the similarity transformed (STEOM-CC) method for excited states in prior work under this grant. This method is the rigorous analog of the convenient and conceptual mono-excited CI method (CIS) but with fully correlated matrix elements, via the similarity transformation that introduces the ground state CC solution and the CC solutions for the ionization potential [(0,1) sector of Fock space] and for electron attachment [(1,0) sector]. Since this method's rate determining step requires being able to perform a ground state CCSD calculation, after a little time for the IP sector and a little more for the EA sector, the excited states obtained are virtually free. Hence, we applied this method to the excited states of free-base porphin in a polarized basis set [5]. This is the largest CC calculation that has been attempted Our results for the excited states appear to be excellent, [5] and this procedure is recommended for studies of a wealth of other excited state problems.

E. One of the more fascinating questions that has arisen in our HEDM studies is whether the O_4 molecule exists in a covalent form, as opposed to the well known Van der Waals dimer $(O_2)_2$. Some calculations have indicated that two forms of a hypothetical O_4 are possible, a cyclic one of D_{2d} symmetry and a 'pin-wheel' form of D_{3h} symmetry. Yet there has been no experimental evidence of their existence. Recently, an interesting experiment was conducted by Suits' *et al.*, who thought they might have seen evidence for a covalent form. The evidence was that O_4^+ ion was seen in the mass spectra, but no O_2^+ signal, which would likely be observed if the origin of the O_4^+ was a Van der Waals complex. Furthermore, there was evidence that one photon was absorbed at about the computed energy of the cyclic form (~4 eV) and a second photon absorbed by a bound excited state at ~4 eV higher. Hence, in collaboration with the experimental group from Berkeley, we used our accurate theoretical methods for ground and excited states to investigate this possibility. However, we found no evidence for a bound excited state ~4 eV above the cyclic form. Furthermore, our computed results for the ionization potential of either of the covalent forms was inconsistent with the observation of O_4^+ formation at the ~12 eV observed in the two-photon experiment [15]. Hence, we concluded, that the experiment was only seeing the Van der Waals form of O_4, [15] despite some unusual aspects to the experiment.

F. We have also characterized the utility of NO_4^+ as a highly energetic species [2] In fact, NO_4^+ would be more powerful than many current oxidizers and its existence is supported by an analogy with NH_4^+ present in ammonium nitrate, NH_4NO_3. Our numerical results showed that NO_4^+ has a bicyclic D_{2d} structure which is 114 kcal mol^{-1} above $NO_2^+ + O_2(^1\Delta_g)$, however the barrier for this process is much too low for handling on a bulk scale. Furthermore, the description of the transition state benefited from our recent methodological development of the double ionization version of the similarity-transformed equation-of-motion method (DIP-STEOM). Unique from other approaches, DIP-STEOM includes important contributions from both dynamic and static correlation in a very economical way. Hence, we provided an upper barrier of 13 kcal mol^{-1} for its unimolecular dissociation and concluded that the lifetime would be very short. There are still open possibilities for the use of short-lived NO_4^+ in the directed synthesis of other molecules and our infrared harmonic frequencies and intensities can aid in its identification.

G. Additional possibilities for highly energetic species are molecules that are composed of solely nitrogen, and a great deal of talent has been directed at producing novel nitrogen species. The repulsion of lone electron pairs on adjacent nitrogen atoms is a strong destabilizing force in these systems and can be reduced if nitrogen forms coordinate covalent bonds with a more electronegative element like oxygen. In recent work, we have considered the differences in structure, energetics, charge distribution and kinetic stability in two series of $(N_2O)_x$ x=2-4 ring systems [42]. In the first series, coordinate covalent bonding exists where the oxygen atom is external to a nitrogen ring. This leads to the long sought N_6 ring analogous to benzene. In the second series, nitrogen-oxygen ring systems of the same stoichiometry are considered for comparison. Although molecules in each series have comparable large positive heats of formation ranging from 117 to 250 kcal mol^{-1}, the coordinate covalent bonded systems have activation barriers to unimolecular dissociation that indicate bulk handling may be possible.

H. In our other major methodological effort we have addressed fundamental elements in density functional theory. In one paper, [21] we have shown that the potential, ie $\delta E_{xc}/\delta\rho(r) = V_{xc}[\rho(r)]$ for the most popular functionals, $E_{xc}[\rho]$, and its kernel, $\delta V_{xc}[\rho(r)]/\delta\rho(r') = f_{xc}[\rho(r')]$ will have the wrong signs for even simple, exact two electron densities. The significance of this result is that without accurate potentials, DFT will not give correct ionization potentials or photoelectron spectra. Furthermore, without getting the correct ionization potentials for **all** the principal ionizations in a molecule, it is impossible to describe Rydberg states properly. If the Rydbergs are wrong, then most of the other excited states are too, since some mixing of Rydbergs with valence states will be essential in a correct description of the latter. In time-dependent Kohn-Sham theory, the results are critically dependent upon the kernel, and in our simple examples that too is shown to have the wrong sign [21].

I. The greatest weakness of DFT in practice is that unlike the established paradigm of CC/MBPT methods where we know that we can converge to the exact answer, there is no way to perform the next higher DFT calculation. Since the method is dependent upon more or less semi-empirically generated potentials, you get what you get, with no way to improve upon the result in a systematic manner. We are working to remove this limitation by doing what we call *ab initio* DFT. As long as we are willing to take functional derivatives wrt to the density via a chain rule that introduces the orbitals used in DFT, and that will also use the 'response' function of DFT, ie $\delta v_s/\delta\rho(r)$, we can build our exchange and our correlation potentials solely from the first principle expressions that we know they have. The exchange is $-\Sigma_{ij}<ij|ji>$ subject to i and j being the Kohn-Sham orbitals. Differentiating wrt to $\rho(r)$, leads us to an integro-differential equation that defines the **exact** exchange potential, V_x. In terms of rigor, this cannot be improved upon by any approximation. We have recently publishd a paper in Physical Review Letters [24] which shows that any of the current correlation potentials when used with the exact exchange overcorrects for the first ionization potential, which should be the eigenvalue of the HOMO in the exact KS theory. This is not surprising, since unlike most DFT being done today, having the exact exchange eliminates fortuitous cancellation of error between the exchange and correlation. We

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have embarked upon similar methods for the exact correlation potential, which can be conveniently defined in terms of KS orbitals in CC theory.

III. Publications Sponsored by AFOSR

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3. S. A. Kucharski and R. J. Bartlett, "Noniterative energy corrections through fifth-order to the coupled cluster singles and doubles method," J. Chem. Phys. **108**, 5243-5254 (1998).
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35. J. Del Bene, and R. J. Bartlett, "N^{-N} spin-spin coupling constants $\left[^{2h}J\left(^{15}N\text{-}^{15}N \right) \right]$ across N-H...N hydrogren bonds in neutral complexes: To what extent does this bonding at the nitrogen influence $^{2h}J_{N\text{-}N}$,?" JACS Communication, in press.

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38. S. Hirata, M. Nooijen, and R. J. Bartlett, "High-order determinantal equation-of-motion coupled-cluster calculations for ionized and electron-attached states," Chem. Phys. Lett., in press.

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40. J. Del Bene, A. Perera, R.J. Bartlett, I, Alkorta, and J. Elguero, $^4J(^{31}P-^{31}P)$ Coupling Constants through N-H+-N Hydrogen Bonds: A Comparison of Computed Ab Initio and Experimental Data," J. Phys. Chem., accepted.

41. S. Ivanov, R.J. Bartlett, "Exact Expression for the Correlation Potential in the High-Density Limit," J. Chem. Phys., Communication, accepted.

42. K. J. Wilson, S. A. Perera, J. D. Watts, and R. J. Bartlett, "Nitrogen-oxygen coordinate covalent bonds: Structural, energetic and stability differences in a series of $(N_2O)_x x$=2-4 ring systems, "J. Phys. Chem., to be submitted.

43. R. J. Bartlett, "Quantum Chemistry in the New Millennium: The Next Step," *Chemistry for the 21st Century*, Edited by: Keinan/Schechter, to be published.

IV. Invited Presentations

August 2000 —"NMR Coupling Constants Across Hydrogen Bonds: The Role of Predictive Theory," University of Tennessee, Knoxville, Tennessee

August 2000 —"NMR Coupling Constants Across Hydrogen Bonds: The Role of Predictive Theory," Oak Ridge National Lab, Tennessee

July 2000 — "Ab Initio Density Functional Theory," 4th Canadian Computational Chemistry Conference, Bishop's University, Lennoxville, Québec, Canada

May 2000 —"Predicted NMR Coupling Constants Across Hydrogen-Bonds: A Fingerprint for Specifying Hydrogen Bond Type?," SETCA 2000, University of Georgia, Athens, GA.

May 2000—"Ab Initio Density Functional Theory," Twelfth Annual Workshop on Recent Developments in Electronic Structure Methods," Georgia Institute of Technology, Atlanta, GA.

April 2000—"Ab Initio Density Functional Theory," Fifth European Workshop on Quantum Systems in Chemistry and Physics, Uppsala, Sweden, April 13-18 2000.

February 2000—"Coupling Constants Across Hydrogen Bonds in NMR: The Role of Predictive Theory," Bircher Lecture, Vanderbilt University, Nashville, TN.

January 2000—"High Energy Density Materials," HEDM/DARPA Meeting, Arlington, VA.

November 1999—"Correlation in Molecules and Solids," The Third Congress of the International Society for Theoretical Chemical Physics, Mexico City, Mexico, November 8-13, 1999.

October 1999—"Excited States in Molecules and Solids. Interplay between Experiment and Theory," ESMS 99 Conference, Tarragona, Spain, October 21-24, 1999.

September 1999—"Computational Methods in Quantum Chemistry," 11th European Seminar on Computational Methods in Quantum Theory, Zakopane, Poland, September 23-25, 1999.

August 1999—"On the Interface of Density Functional Theory with Correlated Ab Initio Methods," American Chemical Society Meeting, New Orleans, LA, August 23-27, 1999.

August 1999—"Nonlinear Optics," American Chemical Society Meeting, New Orleans, LA, August 23-27, 1999.

June 1999—"N_2O Dimers, Trimers and Tetramers: A New Class of Potential HEDM's," Air Force Office of Scientific Research Annual Contractor's Review, Cocoa Beach, FL, June 8-10, 1999.

June 1999—"A Survey of Polynitrogen Systems: N_2-N_8 ," DARPA Meeting, Cocoa Beach, FL, June 11, 1999.

April 1999—"Ab Initio Quantum Chemistry, NMR and Hydrogen Bonds," Distinguished Lecture Series in Computational Chemistry and Physics at Jackson State University, Jackson, MS, May 14, 1999.

March 1999—"Coupled-Cluster Theory, Density Functional Theory, and Excited States," American Physical Society Centennial Meeting, Atlanta, GA, March 20-26, 1999.

January 1999—Meeting of High Energy Density Materials research group at US Air Force, Arlington, VA, January 26-27, 1999.

October 1998—"Response Theory in Density Functional Theory and Coupled-cluster Theory," CECAM (European Centre for Atomic and Molecular Computations) Workshop on Electronic Response Functions in Atoms, Molecules, and Solids, Lyon, France, October 5-7, 1998.

September 1998—"The Coupled-Cluster Treatment of NMR and ESR Spectra," International Conference on Quantum Chemical Calculations of NMR and EPR Parameters, Bratislava-Smolenice, Slovak Republic, September 14-18, 1998.

August 1998—"Twenty Years of Coupled-cluster Theory: Overview and Reflection," Physical Chemistry Division symposium, *A Celebration of 20 Years of the Subdivision of Theoretical Chemistry*, American Chemical Society National Meeting, Boston MA, 23-27 August 1998.

May 1998—"Quantum Chemistry at the Interface of Density Functional Theory and *ab initio* Correlated Methods," 27th Annual Meeting of the Southeastern Theoretical Chemistry Association, The Florida State University, Tallahassee FL.

May 1998—"Does the O_4 Molecule Exist?" 1998 High Energy Density Matter Contractor's Meeting, AFOSR, Monterey CA.

V. Students Supported

Stefan Fau - Postdoc
Ireneusz Grabowski - Postdoc
Thomas Henderson - Graduate Student
So Hirata - Postdoc
Christine Jamorski - Postdoc
Motoi Tobita - Graduate Student
Kenneth Wilson - Graduate Student
Anthony Yau - Graduate Student

VI.   Recognition

A.   Florida Award

2000 Florida Award
Dr. Rodney J. Bartlett, Graduate Research Professor of
Chemistry and Physics, University of Florida, Gainesville,
Florida, is the winner of the 2000 Florida Award

Editor's note: The summary provided here was extracted from the nomination documents submitted by Dr. John R. Eyler of the University of Florida.

Professor Bartlett was born in Memphis, Tennessee in 1944. He lived there through his high school years until attending Millsaps College in Jackson, Mississippi where he received a B.S. degree, with a double major in Chemistry and Mathematics.

He received his Ph.D. degree from the University of Florida in 1971 working with Graduate Research Professor Per-Olov Löwdin and Professor N. Yngve Öhrn. After postdoctoral work at Aarhus University on an NSF postdoctoral fellowship and at John Hopkins University, Dr. Bartlett spent 7 years at Battelle Memorial Institute, first at the Pacific Northwest National Laboratory and then at Battelle in Columbus, Ohio. In 1981 he moved to the University of Florida as Professor of Chemistry and Physics and as a member of the Quantum Theory Project. He was promoted to Graduate Research Professor in 1987. Dr. Bartlett was named a University of Florida Research Foundation Professor in 1998 (a three year award) in recognition of outstanding research and scholarly achievements. He was also named a David L. Williams Term Professor in the College of Liberal Arts and Sciences for 1997-1998. In 1998 he received a University of Florida Professorial Excellence Program (PEP) Award.

Dr. Bartlett is a member of the International Academy of Quantum Molecular Sciencnes (1991), a fellow of the American Physical Society (1986), and has held a Guggenheim Fellowship (1986-1987). He has served during consecutive years in the mid-1980s as chairman-elect-designate, chairman-elect, and chairman of the Subdivision of Theoretical Chemistry of the American Chemical Society. He has organized many symposia,

including four at American Chemical Society National meetings. He regularly has contributed to the organization of the annual Sanibel Symposium run by the Quantum Theory Project. His memberships in honoraries include Phi Beta Kappa, Phi Kappa Phi, Omicron Delta Kappa, and American Men and Women of Science.

Dr. Bartlett has pioneered the development of coupled-cluster theory and many-body perturbation theory in quantum chemistry to offer highly accurate solutions of the Schrödinger equation for molecular structure and spectra that properly include the essential effects of electron correlation. His research interests include: flame chemistry; nonlinear optical properties of molecules; the search for high-energy density molecules, including metastable ones; clusters, particularly those due to carbon, and their role in interstellar space; NMR spectra; exotic anions; and excited, ionized, and electron-attached states of molecules. He is also developing correlated methods for periodic infinite systems like polymers, surfaces, and crystals and is using coupled-cluster methods to develop new exchange-correlation functionals in density functional theory. He maintains a group of a dozen people. He has published over 300 papers and has presented over 100 invited lectures at major meetings. According to the Institute for Scientific Information (Philadelphia, Pennsylvania), he is the 25th most cited chemist in the world for the period from June 1981 through June 1997.

Rod Bartlett has taught undergraduate general and physical chemistry courses and graduate courses in quantum chemistry. His current teaching duties focus on advanced quantum chemistry classes and directing a large research group. During the last several summers, Dr. Bartlett has directed students participating in the NSF-sponsored Research Experiences for Undergraduates Program.

B.   BIRCHER LECTURE - VANDERBILT UNIVERSITY, FEBRUARY 7, 2000

(PLEASE SEE ATTACHED)

C.   ISI's 50 Most Cited Chemists, 1981-1997, ranked by total citations

ISI's 50 Most Cited Chemists, 1981-June 1997,
ranked by total citations:
David A. Pendlebury

Name	Papers 81-June 97	Citations 81-June 97	Cites/Paper (Impact)
1-10			
A.Bax	152	21,655-	142.47
J.A.Pople	176	14,044	79.80
R..R.Ernst [N]	182	13,069	71.81
G.M.Whitesides	318	12,310	38.71
P.V.Schleyer	488	12,171	24.94
H.F.Schaefer	515	11,921	23.15
J.C.Huffman	577	11,654	20.20
A.L.Rheingold	830	11,317	13.63
D.Seebach	349	11,275	32.31
J.M.Lehn [N]	307	10,823	35.25
11-20			
T.J.Meyer	267	10,490	39.29
R.E.Smalley(N)	96	10,456	108.92
A.J.Bard	333	10,365	31.13
D.G.Truhlar	328	10,310	31.43
J.J.P.Stewart	39	10,179	261.00
E.J.Corey (N)	303	10,129	33.43
P.A.Kollman	140	9,703	69.31
M.J.S.Dewar	119	9,701	81.52
W.L.Jorgensen	154	9,695	62.95
R.N.Zare	290	9,617	33.16
21-30			
B.M.Trost	332	9,302	28.02
C.W.Bauschlicher	351	9,139	26.04
A.H.White	866	9,107	10.52
R.Taylor	221	9,020	40.81
▶ **R.J.Bartlett**	**251**	**8,984**	**35.79**
G.A.Somorjai	328	8,958	27.31
K.N.Houk	287	8,654	30.15
T.J.Marks	217	8,366	38.55
S.J.Lippard	230	8,342	36.27
K.Raghavachari	123	8,272	67.25
31-40			
R.Hoffmann (N)	248	8,269	33.34
A.H.Zewail	211	8,208	38.90
J.L.Atwood	348	8,109	23.30
M.B.Hursthouse	659	8,068	12.15